

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 5.94 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.90e-01

Confidence level: 7.64e-01

Nearest Neighbors from the Training Set

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Ethanol

Measured: 1.58

Predicted: 2.24

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1-Propanol

Measured: 3.02

Predicted: 4.69

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Thioacetamide

Measured: 6.03

Predicted: 6.43

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Ethyleneimine

Measured: 6.03

Predicted: 4.17

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Benzene

Measured: 56.2

Predicted: 50.5